

A-05

IMCA-CAT Insertion Device Beamline Upgraded for High-throughput, Shutterless, Continuous-rotation Data Collection

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The IMCA-CAT insertion device beamline, 17-ID, has been upgraded to a microfocused high-flux diffraction beamline for automated high-throughput macromolecular crystallography. The energy range is 6–20 keV, allowing multi-wavelength anomalous dispersion/single-wavelength anomalous dispersion experiments at energies for commonly used derivatives. The full beam is focused to 65 μm \times 30 μm at the sample position and the GM/CA-CAT mini-quad collimators provide the user with selectable beam sizes of 300, 20, 10, and 5 μm . Beam stability is achieved with custom software that automatically positions the beam with 62 μm positional accuracy. Automated sample mounting is performed with the Rigaku ACTOR robot, and samples are viewed with the Maatel on-axis viewing system. The new ALIO goniometer has a small (1.2 μm) sphere of confusion, thus maintaining accurate sample positioning. A new detector, the PILATUS 6M pixel-array from DECTRIS, permits shutterless, continuous-rotation data collection. The high volume of data is managed with a 64 TB storage system that consists of a highly available Lustre-distributed parallel file system with Fibre Channel and InfiniBand interconnects. Custom software provides an intuitive interface for controlling the beamline. Rigaku JDirector software for data collection enables queuing of data collection jobs for automated data acquisition. Both unattended and remote data collection modes are supported. The automated and rapid data collection capabilities of beamline 17-ID are ideally suited for high-throughput crystallography projects such as pharmaceutical industry drug discovery programs.

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